An Investigation into the Effects of Temperature and Crystallization Conditions on the Lattice Parameters of Ultra Long n-alkane Crystals

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Ultra-long, strictly monodisperse n-alkanes, with a chain length between 100 and 400 carbons, crystallize into extremely regular lamellae with a thickness that is an integer fraction of the extended chain length. They have been investigated as model systems for polymer crystallisation, crystal annealing and melting.

High resolution time resolved wide angle X-ray scattering has been performed on beamline ID11 at the ESRF, in Grenoble. Changes in the lattice parameters of a range of ultra long n-alkanes have been determined as a function temperature. Emphasis has been placed on observing the transitions of chain unfolding and melting. The principal component of unit cell expansion is directed along the *a* axis, with little change parallel to the *b* and *c* axes, in agreement with previous studies. Subtle differences in the lattice parameters depending on the crystal thickness and the number of folds in the chain have been observed. At room temperature the number of folds has a controlling influence over the lattice parameters, with the more folded crystals having a more expanded lattice. Crystal thickness starts to play a role as the melting temperature is approached. The effect of pressure on the temperature dependance of lattice parameters in these model systems was also investigated, in the range 0-6 kbar.

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